ON THE DEVELOPMENT OF NUCLEAR DATA FOR LFR

PABLO ROMOJARO OTERO
Research Engineer
SCK CEN

NURIA GARCÍA HERRANZ
Profesora Titular de Universidad
UNIVERSIDAD POLITÉCNICA DE MADRID

FRANCISCO ÁLVAREZ VELARDE
Investigador Científico
CENTRO DE INVESTIGACIONES ENERGÉTICAS, MEDIOAMBIENTALES Y TECNOLÓGICAS (CIEMAT)

INTRODUCTION

The Lead-cooled Fast Reactor (LFR) is one of the three advanced reactor technologies selected by the Sustainable Nuclear Energy Technology Platform [1] that can meet future European energy needs. However, significant drawbacks for the industrial deployment of LFR still exist, among which are the lack of operational experience and the little knowledge about the potential impact of uncertainties in the reactor design, operation and safety assessment.

Traditionally, expensive experimental facilities have been needed for the design of a new nuclear reactor in order to conduct dedicated experiments to cover a wide range of scenarios and aspects of the new system. Nowadays, considering the cost of such facilities, it would be desirable that the design of new systems could rely more on computer simulations. Accurate simulations can help to improve understanding and to optimize the design and safety margins in any operational conditions. Hence, the capability to provide reliable predictions is recognized as a priority to support the development of LFR technologies.

The quantification of uncertainties associated with the computational outcomes is imperative to establish the credibility of the results and make robust decisions based on simulations. In nuclear reactor design, the uncertainties come from material properties, fabrication tolerances, operative conditions, simulation tools and nuclear data. The uncertainty in nuclear data is one of the most important sources of uncertainty in neutronics calculations and consequently in reactor design [2]. Accurate and reliable tools are therefore needed to propagate nuclear data uncertainties to reactor key parameters (neutron multiplication factor, safety coefficients, …).

Significant gaps between the estimated uncertainties in reactor core parameters and the target accuracies (i.e., maximum acceptable uncertainties for a certain parameter) have been systematically shown in the past [3], suggesting nuclear data weaknesses. Meeting the target accuracy is required not only to achieve the requested level of safety for this technology, but also to minimize the increase in the costs due to additional safety measures.

The aim of this article is to present the analyses and work performed to improve the nuclear data required for the development, safety assessment and licensing of LFR reactors, reducing the uncertainties in the criticality safety parameters due to the uncertainties in nuclear data, in order to reach the target accuracies defined by scientific community, industry and regulators.

NUCLEAR DATA

Reliable nuclear structure and reaction data constitute the fundamental building of nuclear physics research and are vital for many other applications. In nuclear physics simulations, two classes of data are required [4]: i) data describing neutron (and sometimes other particle) interactions with the nuclei conforming the system; and ii) data describing nuclear changes in system constituents, as a result of fission, activation or decay. All these data are considered nuclear data.

To produce high quality nuclear data, the life cycle presented in Figure 1 is followed. First, novel experimental nuclear reaction data are obtained with energy dependent measurements. Since it is not possible to measure everything, experimental data are usually completed by theoretical model calculations. Then, evaluators produce evaluated data sets through the process of selection, critical comparison, renor-

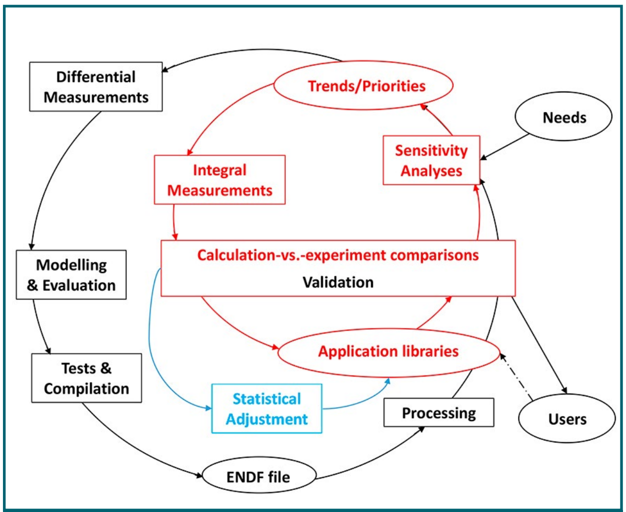

Figure 1. Life cycle of nuclear data [4].

malization and averaging of the available data, to come up with a best judgement of the real values of the underlying nuclear reaction data. Evaluated data are exhaustively tested and verified before their release, in order to ensure that no errors have been made in the evaluation and that the format, in which the data are compiled, is respected. The compendium of such data, usually composed of data for several hundreds of nuclides, is known as evaluated nuclear data libraries, and is written in a specific format called ENDF (Evaluated Nuclear Data File). The processing of nuclear data libraries with specialized computer codes (e.g., NJOY, PREPRO, …), allows obtaining application libraries, which are the input data to computations for a wide variety of nuclear science and technology applications, which need their own format for the nuclear data. Application libraries are validated using integral experimental data, by simulating the integral measurement (e.g., criticality simulation with a transport code such as PARTISN, MCNP, …) and comparing the results from the calculation against the experimental data. Finally, application libraries are employed by users in specific applications (e.g., nuclear reactor design, criticality safety, shielding, medical applications, …). The validation and use of application libraries allow identifying nuclear data needs and establishing nuclear data priorities to perform new measurements or re-evaluations and, thus, the cycle is once again repeated.

It is important to notice that nuclear data are not free of uncertainties due to limitations of measurement procedures, as well as due to uncontrollable statistical fluctuations. Numerical values for physical parameters predicted by theoretical models are also uncertain [5]. These uncertainties are given within the nuclear data evaluations in the form of covariance matrices. However, uncertainties are not always provided and when they are, they may be incomplete or exhibit lack of consistency.

As of the mid-1960s many nuclear data libraries existed. Each laboratory had its own data library, in its own format for its own computer codes, which was designed to get the "best" answers using the in-house laboratory computer codes, for the specific applications that each laboratory was interested in. This often required nonphysical "fixes" or fits to force agreement between computer code and experimental results [6].

On the mid-1960s, an effort began to establish a nuclear data library, containing evaluated data based solely on the "best" available energy dependent measurements and nuclear model calculations. It was hoped that one common library of data could be universally adopted for use throughout the world [6]. Unfortunately, this goal has not been achieved yet and significant differences between the important evaluations in these various data libraries still exist (e.g., JEFF, ENDF/B, JENDL, TENDL, BRONDL,…). This work is focused on the Joint Evaluated Fission and Fusion (JEFF) nuclear data library, which is produced by a coordinated group of the Nuclear Energy Agency (NEA), that belongs to the Organisation for Economic Co-operation and Development (OECD). The latest version, JEFF-3.3 [7], was officially released in November 2017.

JEFF-3.3 NUCLEAR DATA LIBRARY

Before nuclear data can be used for practical applications, a thorough verification/validation must be performed in order to ensure that the data is consistent with energy dependent and integral experimental measurements [8]. Therefore, a thorough validation, verification and benchmarking of the latest version of the JEFF library at the time, JEFF-3.3T1, released on March 2016, was performed in order to ensure the

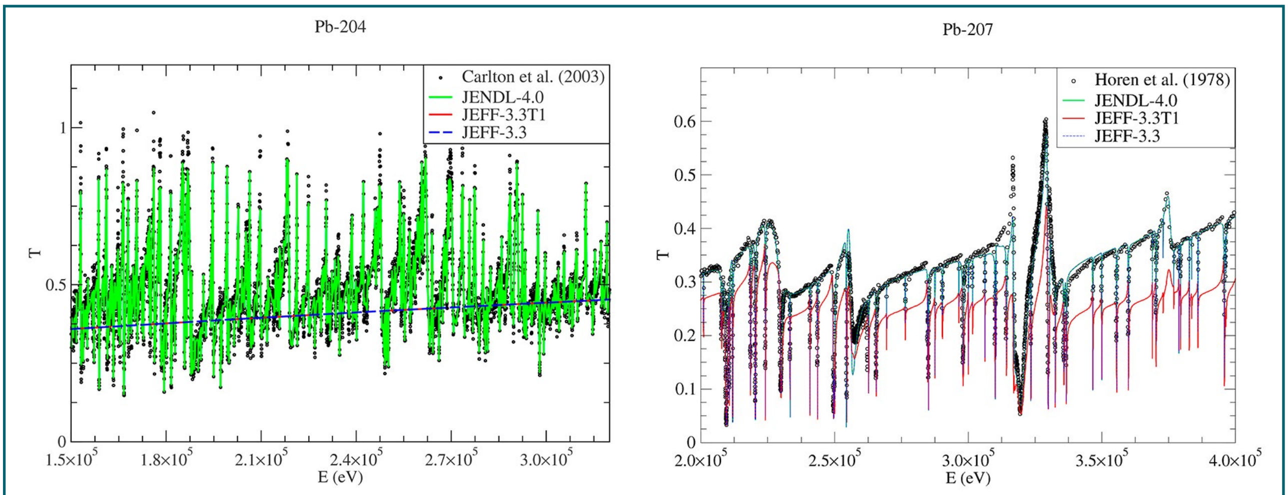

Figure 2. ^{204}Pb (left) and ^{207}Pb (right) transmission comparisons with experimental data.

quality and accuracy of the data used in the posterior analyses. In particular, the coolant materials of an LFR, lead and bismuth, were chosen as the main objects of study since they are of vital importance for the neutronics performance and criticality safety, and were not covered in the CIELO pilot project [9].

Several problems were found in the Resolved and Unresolved Resonance Ranges (RRR and URR) of JEFF-3.3T1 lead and bismuth files: in ^{204}Pb the total cross section is underestimated due to the lack of resonances (Figure 2); the total cross section of ^{207}Pb is severely overestimated (underestimation of the transmission); and ^{209}Bi overestimates the total cross section in the RRR (up to 100 keV) and has a clearly unphysical cross section shape from 100 to 250 keV, missing resonances at the upper end of the RRR (from 100 to 200 keV) and providing only background (Figure 3).

These problems, as well as the recommendation to employ the RRR from JENDL-4.0 for these isotopes in the final version of JEFF-3.3, were communicated to the JEFF collaboration [10] and, as it can be seen in Figure 2 and Figure 3, the recommendations were adopted in the production version of JEFF-3.3 nuclear data library, excepting for ^{204}Pb which is still based on JEFF-3.2 evaluation.

While numerous integral benchmarks sensitive to lead isotopes have been found in the criticality and reactor databases, a lack of integral benchmarks with enough sensitivity to bismuth cross sections has been observed and only one benchmark is currently available for bismuth data validation. JEFF-3.3T1 lead evaluation disagrees with all lead integral benchmarks in the RRR and URR energy ranges, whereas bismuth evaluation is not compatible with the transmission benchmark experimental data from 100 to 250 keV due to ^{209}Bi unphysical evaluation. Better agreement is observed for JENDL-4.0 and JEFF-3.3 lead and bismuth evaluations with integral experiments, as it can be seen in Figure 4.

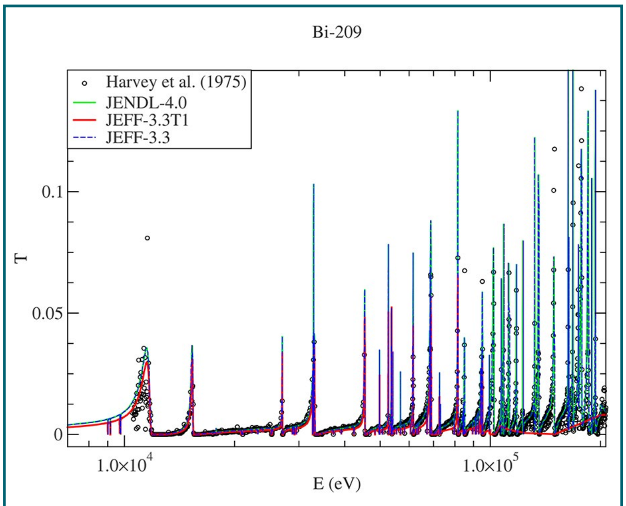

Figure 3. ^{209}Bi transmission comparison with experimental data in the RRR and URR.

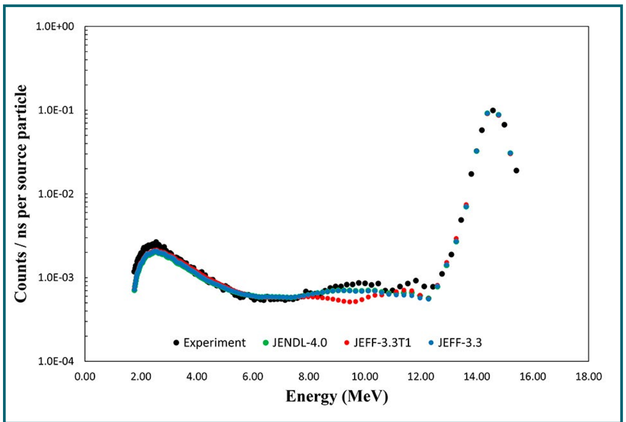

Figure 4. Neutron spectrum for LLNL Pb pulsed sphere.

Once the production version of the JEFF-3.3 nuclear data library was released, JEFF-3.3 lead and bismuth evaluations exhibited better agreement with differential and integral experimental data than JEFF-3.3T1; therefore, they can be considered as a significant improvement over the first beta evaluations for these materials in JEFF-3.3T1.

TARGET ACCURACY ASSESSMENT

Target accuracy assessments (TAA) consist on evaluating the calculated uncertainties against the reactor design target accuracies. They allow identifying nuclear data needs and requirements (by isotope, nuclear reaction and energy channel), in order to reduce margins, achieving the requested level of safety and minimizing the increase in the costs due to additional safety measures, in the preliminary conceptual design and in later design phases of selected reactor and fuel cycle concepts. In Table 1, target accuracies established by researchers and industry for fast reactors at Beginning of Life are presented.

Multiplication Factor	300 pcm
Delayed neutron fraction	3%
Reactivity coefficients (coolant void and Doppler)	7%

Table 1. Fast reactor target accuracies [11,12].

Due to limitations of existing codes, Sensitivity and Uncertainty Methodology for MONtecarlo codes (SUMMON) system has been developed to perform complete automated sensitivity and uncertainty analyses of the most relevant criticality safety parameters of detailed complex reactor designs from the neutronics point of view, i.e., k_{eff}, β_{eff}, Λ_{eff} and reactivity coefficients, using state-of-the-art nuclear data libraries and covariances.

SUMMON is based on the use of the KSEN card of MCNP code to perform the eigenvalue sensitivity calculations, although any code that can provide sensitivity coefficients can be used. The sensitivity coefficients of a reactivity response are calculated using the eigenvalue definition of reactivity, which is equivalent to applying the Equivalent Generalized Perturbation Theory. Moreover, the effective delayed neutron fraction sensitivity coefficients are derived from Bretscher's approximation or employing Chiba's modified method, whereas the sensitivity coefficients of the effective neutron generation time are obtained using the $1/v$ insertion method and the Equivalent Generalized Perturbation Theory. Uncertainties are propagated using the "Sandwich Rule" of the "Propagation of Moments" method employing state-of-the-art covariance libraries [13,14].

The sensitivity coefficient implementations in SUMMON have been validated and verified using integral benchmark experiments from the International Handbook of Evaluated

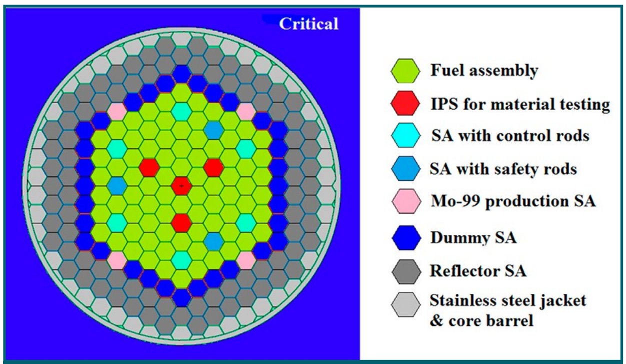

Figure 5. Critical MYRRHA core layout [17].

Criticality Safety Benchmark Experiments (ICSBEP) [13] and comparing SUMMON with the well-validated and consolidated codes such as SCALE, SUSD3D and SERPENT [14,15].

SUMMON system has been used to perform a complete TAA of an advanced LFR-representative, employing the state-of-the-art JEFF-3.3 nuclear data library. MYRRHA experimental reactor has been chosen as the main object of study, due to the key role it will play in the development of the Pb-alloy technology needed for the LFR Generation-IV concept [16] as an LFR pilot plant.

Furthermore, strong support has been given by the Belgian government and numerous countries and, in fact, MYRRHA's project phase 1 has already started with the construction of the 100 MeV particle accelerator and with the pre-licensing of the reactor. For the analyses a simplified model [17], homogenised on fuel assembly level, of the critical core configuration in nominal conditions at Beginning of Life has been used. The layout of the core is shown in Figure 5.

Parameter	Uncertainty (%)
k_{eff}	0.8
β_{eff}	1.1
Doppler coefficient (+400 K)	9.1
Coolant density coefficient (-5%)	20.3
Control rod worth	1.8

Table 2. Uncertainty quantification for MYRRHA with JEFF-3.3.

Sensitivity coefficients and total uncertainties and main contributors to the uncertainty in the criticality safety coefficients have been obtained. In Table 2, global results from the uncertainty quantification analyses are presented. As it can be seen, target accuracies are exceeded for k_{eff}, change in fuel temperature and change in coolant density scenarios. ^{238}U, ^{239,240}Pu, ^{10}B(n,n'), ^{54,56,57}Fe(n,n) and ^{208}Pb(n,n) have been identified as major contributors to the uncertainty in the integral safety-related parameters, due to the high sensitivity of the parameters to these isotopes and/or due to the uncertainty in the cross sections.

DATA ASSIMILATION

To achieve the goal of reducing nuclear data uncertainties in LFR safety coefficients, a reduction of nuclear data uncertainties in JEFF-3.3 for the quantities identified in the TAA is needed. Thus, Data Assimilation With summoN (DAWN) module [18] has been developed to perform data assimilation using integral experiments from public databases, with the aim of providing adjusted nuclear data, not only capable of predicting reactor properties within the target design accuracy, but also statistically consistent with the various differential measurements.

The implemented methodology is based on the Generalised Least Squares technique and the use of integral experiments from ICSBEP database. Individual adjustments using a single experiment or complete adjustments, using up to 93 criticality mass experiments with reported final experimental uncertainties in the ICSBEP Handbook, can be performed.

It must be stressed that, from a general-purpose library, the adjustment procedure generates a specific-application library, only usable for the targeted reactor concept, or for a system with a representativity factor close to one with that targeted reactor or experiments used in the adjustment.

DAWN was then used to perform data assimilation for MYRRHA with JEFF-3.3 nuclear data library on ^{238}U, ^{239,240}Pu, ^{10}B, Fe and Pb isotopes and six experiments selected from ICSBEP. The adjusted nuclear data was then used to re-assess the total uncertainty in k_{eff}, Doppler and coolant density reactivity coefficients (Table 3). The total uncertainty in the reactor parameters has been reduced but target accuracies are still not met. Since the most significant adjustments and anticorrelations were generated for ^{240}Pu and ^{239}Pu, the strongest decrease in uncertainty using the adjusted covariance data concerned k_{eff} (nearly ~300 pcm). On the other hand, the reduction in the reactivity coefficients uncertainty due to the adjustment of iron and lead cross sections can be considered negligible.

Parameter	Posterior uncertainty (%)
k_{eff}	0.5
Doppler coefficient	8.7
Coolant density coefficient	19.5

Table 3. Uncertainty quantification for MYRRHA with adjusted data.

CONCLUSIONS

SUMMON system and DAWN module have been developed to perform sensitivity and uncertainty analyses of reactor criticality safety parameters and constrain uncertainties by means of data assimilation. They allow analysing and improving the nuclear data required for the development, safety assessment and licensing of lead cooled fast reactors, reducing the uncertainties in the criticality safety parameters due to the uncertainties in nuclear data, in order to reach the target accuracies defined by industry, experts and regulators.

Several problems were found in the RRR of JEFF-3.3T1 lead and bismuth. These problems, as well as the recommendation to employ the RRR from JENDL-4.0 for these nuclides in the final version of JEFF-3.3, were communicated to the JEFF collaboration and the recommendations were adopted in the production version of JEFF-3.3 nuclear data library.

A TAA of the latest MYRRHA design has been performed with the SUMMON system and JEFF-3.3 nuclear data library, showing that the target accuracies defined by researchers, industry and experts for k_{eff}, Doppler and coolant density effects are exceeded.

Aiming to produce a new covariance data set capable of predicting the criticality safety coefficients with uncertainties lower than the established target accuracies, SUMMON's data assimilation module, DAWN, has been used to perform data assimilation. While a significant reduction in k_{eff} uncertainty was observed, k_{eff}, Doppler and coolant density coefficients target accuracies were still not met. However, it was proved that the combination of experimental covariance data and integral experiments together with Generalised Least Squares technique, can provide adjusted nuclear data capable of predicting reactor properties with lower uncertainty and consistent with differential data.

Finally, as a result of this work, measurements to produce experimental transmission data that can be used to validate evaluated cross sections for neutron induced reactions on ^{nat}Pb and ^{209}Bi in the resonance region have been proposed.

BIBLIOGRAPHY

[1]. Sustainable Nuclear Energy Technology Platform. http://www.snetp.eu/. Accessed: 15-06-2020.

[2]. I. Kodeli. Sensitivity analysis and uncertainty propagation from basic nuclear data to reactor physics and safety relevant parameters. Workshop Proceedings of Evaluation of uncertainties in relation to severe accidents and level-2 probabilistic safety analysis; Aix-en-Provence, France, 7-9 November 2005. OECD/NEA (2007).

[3]. A.J.M. Plompen and H. Harada. Meeting Nuclear Data Needs for Advanced Reactor Systems. OECD/NEA Report NEA/NSC/WPEC/DOC(2014)446 (2014).

[4]. A.J. Koning et al. Status of the JEFF nuclear data library. J. Korean Phys. Soc. 59 (2011) 1057-1062.

[5]. D.L. Smith and N. Otuka. Experimental Nuclear Reaction Data Uncertainties: Basic Concepts and Documentation. Nucl. Data Sheets 113 (2012) 3006-3053.

[6]. D.G. Cacuci. Handbook of Nuclear Engineering. Springer Science & Business (2010).

[7]. A.J.M. Plompen et al. The Joint Evaluated Fission and Fusion Nuclear Data Library, JEFF-3.3. Eur. Phys. J. (2020). Accepted for publication.

[8]. A. Trkov. Status and Perspective of Nuclear Data Production, Evaluation and Validation. Nucl. Eng. Technol. 37 (2005) 11-24.

[9]. M.B. Chadwick et al. CIELO Collaboration Summary Results: International Evaluations of Neutron Reactions on Uranium, Plutonium, Iron, Oxygen and Hydrogen. Nucl. Data Sheets 148 (2018) 189-213.

[10]. P. Romojaro and F. Alvarez-Velarde. JEFF-3.3T1 processing & testing for ASTRID and MYRRHA. OCDE/NEA Nuclear Data Week, Paris, France, 25-28 April (2016).

[11]. M. Salvatores and R. Jacqmin. Uncertainty and target accuracy assessment for innovative systems using recent covariance data evaluations. OECD/NEA Report NEA/WPEC-26 (2008).

[12]. A. D'Angelo and J.L. Rowlands. Conclusions concerning the delayed neutron data for the major actinides. Prog. Nucl. Energy 41, (2002) 391-412.

[13]. OECD/NEA. International Handbook of Evaluated Criticality Safety Benchmark Experiments. OECD/NEA Report NEA/NSC/DOC(95)03 (2019).

[14]. P. Romojaro et al. SUMMON: A Sensitivity And Uncertainty Methodology For MONte Carlo Codes. M&C 2017, Jeju, Korea, 16-20 April (2017).

[15]. P. Romojaro et al. Sensitivity methods for effective delayed neutron fraction and neutron generation time with SUMMON. Ann. Nucl. Energy 126 (2019) 410-418.

[16]. G. Van den Eynde et al. An updated core design for the multi-purpose irradiation facility MYRRHA. J. Nucl. Sci. Technol. 52 (2015) 1053-1057.

[17]. A. Stankovskiy and G. Van den Eynde. Neutronic model of MYRRHA design revision 1.6. SCK•CEN Report SCK•CEN/4463803 (2014).

[18]. P. Romojaro et al. Nuclear data analyses for improving the safety of advanced lead-cooled reactors. Eur. Phys. J. WoC 211 (2019) 05002.■